

Application No. 09/595,005

RD-27442

Amendments to the Claims

This listing of claims will replace all prior versions and listings of claims in the application:

Listing of Claims

1. (currently amended) A method to identify improved catalytic mixture entities, comprising steps of:

(A) forming a first population of catalytic mixture entities and detecting a catalytic property of each of said mixture entities by a high throughput screening (HTS) method and

(B) executing a genetic algorithm based on said property of said entities to identify a second population of entities.

2. (original) The method of claim 1, wherein said step (B) comprises at least one operation selected from (i) mutation, (ii) crossover, (III) mutation and selection (iv) crossover and selection and (v) mutation, crossover and selection.

3. (previously presented) The method of claim 1, comprising randomly identifying said first population of entities prior to forming said first population according to step (A).

4. (original) The method of claim 1, further comprising generating a binary string representing said first population of entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

5. (original) The method of claim 1, further comprising generating a binary string representing variable parameters of said first population of entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

6. (previously presented) The method of claim 1, further comprising

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generating a binary string representing variable parameters of entities, forming said entities and selecting said first population from said entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

7. (previously presented) The method of claim 1, further comprising generating a binary string representing variable parameters of entities, forming said entities, evaluating said entities for a desired property, weighting said entities according to an hierarchy of fitness of said property and selecting said first population as a sampling from said weighed entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

8. (previously presented) The method of claim 1, further comprising generating a binary string representing variable parameters of entities, forming said entities, evaluating said entities for a desired property, pairing said entities and (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

9. (previously presented) The method of claim 1, further comprising generating a binary string representing variable parameters of entities, forming said entities, evaluating said entities for a desired property and pairing said entities and (B) comprises executing a genetic algorithm comprising a uniform random crossover operator to produce a binary string representing said second population of entities.

10. (previously presented) The method of claim 1, further comprising generating a binary string representing variable parameters of entities, forming said entities, evaluating said entities for a desired property, weighting said entities according to an hierarchy of fitness according to said property, selecting said first population as a sampling from said weighed entities and pairing said entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

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11. (original) The method of claim 1, further comprising conducting steps (A) and (B) on said second population of entities to produce a third population of entities.

12. (original) The method of claim 1, further comprising repeating steps (A) and (B) on said second population of entities and subsequent populations of entities until a fit entity is identified.

13. (canceled)

14. (canceled)

15. (original) The method of claim 1, wherein said HTS method is a combinatorial organic synthesis (COS).

16. (original) The method of claim 1, wherein said first population of entities is a catalyst system.

17. (original) The method of claim 1, wherein said first population of entities is a catalyst system comprising a Group VIII B metal.

18. (original) The method of claim 1, wherein said first population of entities is a catalyst system comprising palladium.

19. (original) The method of claim 1, wherein said first population of entities is a catalyst system comprising a halide composition.

20. (original) The method of claim 1, wherein said first population of entities is a catalyst system that includes an inorganic co-catalyst.

21. (original) The method of claim 1, wherein said first population of entities is a catalyst system that includes a combination of inorganic co-catalysts.

22. (currently amended) A high throughput screening (HTS) method to identify entities of an improved catalyst system, comprising:

(A) depositing each of a first population of entities in respective wells of an

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array, wherein the first population of entities is a catalyst system comprising a Group VIII B metal;

- (B) reacting said population to form a plurality of products;
- (C) detecting a property of each of said plurality of products; and
- (D) executing a genetic algorithm based on said property of said plurality of products to identify a second population of entities with favorable catalytic properties.

23. (original) The method of claim 22, further comprising:

- (E) depositing each of said second population of entities in respective wells of an array; and
- (F) reacting said second population to form a second plurality of products.

24. (original) The method of claim 22, comprising randomly identifying said first population of entities prior to depositing said first population according to step (A).

25. (presently amended) The method of claim 22, wherein said step (D) comprises an at least one operation selected from (i) mutation, (ii) crossover, ~~(iii)~~ (iii) mutation and selection (iv) crossover and selection and (v) mutation, crossover and selection.

26. (original) The method of claim 22, further comprising generating a binary string representing said first population of entities and step (D) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

27. (original) The method of claim 22, wherein said HTS method is a combinatorial organic synthesis (COS).

28. (canceled)

29. (canceled)

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30. (original) The method of claim 22, wherein said first population of entities is a catalyst system comprising palladium.

31. (original) The method of claim 22, wherein said first population of entities is a catalyst system comprising a halide composition.

32. (original) The method of claim 22, wherein said first population of entities is a catalyst system that includes an inorganic co-catalyst.

33. (original) The method of claim 22, wherein said first population of entities is a catalyst system that includes a combination of inorganic co-catalysts.

34. (canceled)

35. (canceled)

36. (canceled)

37. (canceled)

38. (canceled)

39. (canceled)

40. (currently amended) A method of ~~selecting a~~ identifying a prospective carbonylation catalyst, comprising:

(A) forming a first population of prospective carbonylation catalyst entities and detecting a property of each of said entities; and

(B) executing a genetic algorithm based on said property of said entities to identify a second population of prospective carbonylation catalyst entities with favorable properties.

41. (canceled)

42. (new) The method of claim 40, wherein said step (B) comprises at least

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one operation selected from (i) mutation, (ii) crossover, (iii) mutation and selection (iv) crossover and selection and (v) mutation, crossover and selection.

43. (new) The method of claim 40, comprising randomly identifying said first population of entities prior to forming said first population according to step (A).

44. (new) The method of claim 40, further comprising generating a binary string representing said first population of entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

45. (new) The method of claim 40, further comprising generating a binary string representing variable parameters of said first population of entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

46. (new) The method of claim 40, further comprising generating a binary string representing variable parameters of entities, forming said entities and selecting said first population from said entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

47. (new) The method of claim 40, further comprising generating a binary string representing variable parameters of entities, forming said entities, evaluating said entities for a desired property, weighting said entities according to an hierarchy of fitness of said property and selecting said first population as a sampling from said weighed entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

48. (new) The method of claim 40, further comprising generating a binary string representing variable parameters of entities, forming said entities, evaluating said entities for a desired property, pairing said entities and (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

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49. (new) The method of claim 40, further comprising generating a binary string representing variable parameters of entities, forming said entities, evaluating said entities for a desired property and pairing said entities and (B) comprises executing a genetic algorithm comprising a uniform random crossover operator to produce a binary string representing said second population of entities.

50. (new) The method of claim 40, further comprising generating a binary string representing variable parameters of entities, forming said entities, evaluating said entities for a desired property, weighting said entities according to an hierarchy of fitness according to said property, selecting said first population as a sampling from said weighed entities and pairing said entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

51. (new) The method of claim 40, further comprising conducting steps (A) and (B) on said second population of entities to produce a third population of entities with more favorable catalytic properties.

52. (new) The method of claim 40, further comprising repeating steps (A) and (B) on said second population of entities and subsequent populations of entities until a fit entity is identified.

53. (new) The method of claim 40, wherein said first population of entities is formed by steps of:

providing a first reactant system at least partially embodied in a liquid; and

contacting the liquid with a second reactant system at least partially embodied in a gas, the second reactant system having a mass transport rate into the liquid wherein the liquid forms a film having a thickness sufficient to allow a reaction rate that is independent of the mass transport rate of the second reactant system into the liquid to form said first population of entities.

54. (new) The method of claim 40, wherein said method is a combinatorial

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organic synthesis (COS).

55. (new) The method of claim 40, wherein said first population of prospective carbonylation catalyst entities is a catalyst system.

56. (new) The method of claim 40, wherein said first population of prospective carbonylation catalyst entities is a catalyst system comprising a Group VIII B metal.

57. (new) The method of claim 40, wherein said first population of prospective carbonylation catalyst entities is a catalyst system comprising palladium.

58. (new) The method of claim 40, wherein said first population of prospective carbonylation catalyst entities is a catalyst system comprising a halide composition.

59. (new) The method of claim 40, wherein said first population of prospective carbonylation catalyst entities is a catalyst system that includes an inorganic co-catalyst.

60. (new) The method of claim 40, wherein said first population of prospective carbonylation catalyst entities is a catalyst system that includes a combination of inorganic co-catalysts.

61. (new) A method to identify improved mixture entities, comprising steps of:

(A) forming a first population of mixture entities and detecting a catalytic property of each of said entities by a high throughput screening (HTS) method comprising providing a first reactant system at least partially embodied in a liquid and contacting the liquid with a second reactant system at least partially embodied in a gas, the second reactant system having a mass transport rate into the liquid wherein the liquid forms a film having a thickness sufficient to allow a reaction rate that is independent of the mass transport rate of the second reactant system into the liquid; and

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(B) executing a genetic algorithm based on said property of said entities to identify a second population of entities with favorable properties.

62. (new) The method of claim 61, wherein said step (B) comprises at least one operation selected from (i) mutation, (ii) crossover, (iii) mutation and selection (iv) crossover and selection and (v) mutation, crossover and selection.

63. (new) The method of claim 61, comprising randomly identifying said first population of entities prior to forming said first population according to step (A).

64. (new) The method of claim 61, further comprising generating a binary string representing said first population of entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

65. (new) The method of claim 61, further comprising generating a binary string representing variable parameters of said first population of entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

66. (new) The method of claim 61, further comprising generating a binary string representing variable parameters of entities, forming said entities and selecting said first population from said entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

67. (new) The method of claim 61, further comprising generating a binary string representing variable parameters of entities, forming said entities, evaluating said entities for a desired property, weighting said entities according to an hierarchy of fitness of said property and selecting said first population as a sampling from said weighed entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

68. (new) The method of claim 61, further comprising generating a binary

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string representing variable parameters of entities, forming said entities, evaluating said entities for a desired property, pairing said entities and (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

69. (new) The method of claim 61, further comprising generating a binary string representing variable parameters of entities, forming said entities, evaluating said entities for a desired property and pairing said entities and (B) comprises executing a genetic algorithm comprising a uniform random crossover operator to produce a binary string representing said second population of entities.

70. (new) The method of claim 61, further comprising generating a binary string representing variable parameters of entities, forming said entities, evaluating said entities for a desired property, weighting said entities according to an hierarchy of fitness according to said property, selecting said first population as a sampling from said weighed entities and pairing said entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

71. (new) The method of claim 61, further comprising conducting steps (A) and (B) on said second population of entities to produce a third population of entities with more favorable properties.

72. (new) The method of claim 61, further comprising repeating steps (A) and (B) on said second population of entities and subsequent populations of entities until a fit entity is identified.

73. (new) The method of claim 61, wherein said HTS method is a combinatorial organic synthesis (COS).

74. (new) The method of claim 61, wherein said first population of entities is a catalyst system.

75. (new) The method of claim 61, wherein said first population of entities is

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a catalyst system comprising a Group VIII B metal.

76. (new) The method of claim 61, wherein said first population of entities is a catalyst system comprising palladium.

77. (new) The method of claim 61, wherein said first population of entities is a catalyst system comprising a halide composition.

78. (new) The method of claim 61, wherein said first population of entities is a catalyst system that includes an inorganic co-catalyst.

79. (new) The method of claim 61, wherein said first population of entities is a catalyst system that includes a combination of inorganic co-catalysts.